

2,2,3,3,4,4,5,5,6,7,7,7-Dodecafluoro-6-(trifluoromethyl)heptanoic acid
15166-06-0 | DTXSID50562865

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.10

Global applicability domain: Inside

Local applicability domain index: 9.82e-01

Confidence level: 7.26e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Pyrrolidine</div> <div>Measured: 4.07</div> <div>Predicted: 4.10</div>	<div>Image not found</div> <div>Butylamine</div> <div>Measured: 3.61</div> <div>Predicted: 4.09</div>	<div>Image not found</div> <div>1-Butanol</div> <div>Measured: 4.19</div> <div>Predicted: 4.03</div>
<div>Image not found</div> <div>Isopentyl alcohol</div> <div>Measured: 4.52</div> <div>Predicted: 4.24</div>	<div>Image not found</div> <div>2-Chloroethanol</div> <div>Measured: 4.30</div> <div>Predicted: 4.07</div>	